Supplemental Information:
Chemical Composition of Gas- and Aerosol-Phase Products from the Photooxidation of Naphthalene

K. E. Kautzman, J. D. Surratt, M. N. Chan, A. W. H. Chan, S. P. Hersey, P. S. Chhabra, N.F. Dalleska, P. O. Wennberg, R. C. Flagan, and J. H. Seinfeld

Number of Pages: 38
Number of Tables: 7
Number of Figures: 4

TABLE 1S: List of Chemicals Used.

compound	elemental composition	MW (g mol^{-1})	purity (%)
2-Hydroxycinnamic Acid	$C_9H_8O_3$	164	97
1,2,4-benzenetricarboxylic Acid	$C_9H_6O_6$	210	99+
3-Formylbenzoic Acid	$C_8H_6O_3$	150	97
3-Hydroxy-4-Nitrobenzoic Acid	$C_7H_5NO_5$	183	>97
Phthaldialdehyde	$C_8H_6O_2$	134	>97
Phthalic Acid	$C_8H_6O_4$	166	>99.5
Terephthalic Acid	$C_8H_6O_4$	166	98
3,6-Dihydroxy Phthalic Acid	$C_8H_6O_6$	198	n/a
2-Nitrophenol	$C_6H_5NO_3$	139	98
trans-Cinnamic Acid	$C_9H_6O_2$	148	99+
4-Formylcinnamic Acid, *trans*	$C_{10}H_8O_3$	176	n/a
5-Hydroxyisophthalic Acid	$C_8H_6O_5$	182	97
4-Methoxyisophthalic Acid	$C_9H_8O_5$	196	97
4-nitro-1-napthol	$C_{10}H_7NO_3$	189	99
2-nitro-1-napthol	$C_{10}H_7NO_3$	189	99
Benzoic Acid	$C_7H_6O_2$	122	>99.5
3-Hydroxybenzoic Acid	$C_7H_6O_3$	138	>99
Naphthalene	$C_{10}H_8$	128	99
1-Napthol	$C_{10}H_8O$	144	99
Glycolic Acid	$C_2H_4O_3$	76	99
Malic Acid	$C_4H_6O_5$	134	99+
Oxalic Acid	$C_2H_4O_4$	90	99+
Succinic Acid	$C_4H_6O_4$	118	99+
Pyruvic Acid	$C_3H_4O_3$	88	98
Formic Acid	CH_2O_2	46	91
Salicylic Acid	$C_7H_6O_3$	138	99+
Malonic Acid	$C_3H_4O_4$	104	99
Glutaric Acid	$C_5H_8O_4$	132	99
Adipic Acid	$C_6H_{10}O_4$	146	>99.5

TABLE 2S: SOA Constituents Characterized from a High-NO_x Naphthalene (Experiment 6)[a]

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
121	4.14	121.0301	$C_7H_5O_2^-$	1.1	2.5	[e]	benzoic acid (RT = 5.74 min)	0.89	1.7
	5.44	121.0293	$C_7H_5O_2^-$	0.3	0.3				
	5.71[d]	121.0267	$C_7H_5O_2^-$	-2.3	16.6				
133	5.21	133.3020	$C_8H_5O_2^-$	1.2	15.8	[e]	[f]		
137	4.48	137.0253	$C_7H_5O_3^-$	1.4	3.4	93 ($-CO_2$)[g]	3-hydroxybenzoic acid (RT = 6.27 min)	1.01	1.9
	5.30	137.0228	$C_7H_5O_3^-$	-1.1	2.1				
	6.25	137.0255	$C_7H_5O_3^-$	1.6	10.8				
	7.18[d]	137.0222	$C_7H_5O_3^-$	-1.7	3.8				
138	6.21	138.0225	$C_6H_4NO_3^-$	3.4	1.3	[e]	2-nitrophenol (RT = 7.28 min)	0.56	1.1
	6.84[d]	138.0179	$C_6H_4NO_3^-$	-1.2	1.0				
	7.39	138.0198	$C_6H_4NO_3^-$	0.7	0.9				
143	8.75[d]	143.0531	$C_{10}H_7O_1^-$	3.4	1.8	[e]	[f]		
	8.92	143.0536	$C_{10}H_7O_1^-$	3.9	3.4				
147	6.52[d]	147.0432	$C_9H_7O_2^-$	-1.4	2.5	[e]	*trans*- cinnamic acid (RT = 8.49 min)	0.16	0.3
	6.70	147.0473	$C_9H_7O_2^-$	2.7	2.0				
	7.76	147.048	$C_9H_7O_2^-$	3.4	2.3				
149	4.14	149.0231	$C_8H_5O_3^-$	-0.8	2.4	121 (-CO) 107 105 ($-CO_2$)[g]	3-formylbenzoic acid (RT = 6.81 min)	0.74	1.4
	5.91	149.0241	$C_8H_5O_3^-$	0.2	5.9				
	6.07[d]	149.0239	$C_8H_5O_3^-$	0.0	18.7				
	6.46	149.0248	$C_8H_5O_3^-$	0.9	29.0				

TABLE 2S: continued

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
154	6.62	154.0130	$C_6H_4NO_4^-$	-1.0	2.6	[e]	2-nitrophenol (RT = 7.28 min)	0.42	0.79
159	6.50	159.0454	$C_{10}H_7O_2^-$	0.8	265.0	[e]	[f]		
	7.30	159.0466	$C_{10}H_7O_2^-$	2.0	76.6				
	7.58	159.0476	$C_{10}H_7O_2^-$	3.0	107.0				
	8.01	159.0468	$C_{10}H_7O_2^-$	2.2	107.8				
	8.17[d]	159.0470	$C_{10}H_7O_2^-$	2.4	34.8				
163	5.38	163.0391	$C_9H_7O_3^-$	-0.4	5.1	135 (-CO) 145 ($-H_2O$) 119 ($-CO_2$)[g]	2-hydroxycinnamic acid (RT = 7.68 min)	0.63	1.2
	5.67	163.0366	$C_9H_7O_3^-$	-2.9	2218.1				
	5.96	163.0417	$C_9H_7O_3^-$	2.2	236.8				
	6.69	163.0409	$C_9H_7O_3^-$	1.4	30.0				
	6.80[d]	163.0385	$C_9H_7O_3^-$	-1.0	9.5				
	7.44	163.0407	$C_9H_7O_3^-$	1.2	2.8				
165	5.45	165.0181	$C_8H_5O_4^-$	-0.7	4.2	138 121 ($-CO_2$)[g]	phthalic acid (RT = 5.72 min)	1.78	3.3
	5.69[d]	165.0148	$C_8H_5O_4^-$	-4.0	48.1				
173	4.06	172.9902	$C_6H_5O_4S^-$	-0.7	2.5	109 ($-SO_2$) 93 ($-SO_3$)[g] 80	4-hydroxybenzene sulfonic acid (RT = 0.92)[h]	0.29	0.5
173	7.48	173.0252	$C_{10}H_5O_3^-$	1.3	43.5	155 ($-H_2O$) 145 (-CO)[g] 111	[f]		
	7.73[d]	173.0270	$C_{10}H_5O_3^-$	3.1	66.2				
	8.92	173.0287	$C_{10}H_5O_3^-$	4.8	16.7				
	8.99	173.0267	$C_{10}H_5O_3^-$	2.8	59				

TABLE 2S: continued

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
175	6.90[d]	175.0377	$C_{10}H_7O_3^-$	-1.8	43.7	147 (-CO)[g] 131 ($-CO_2$)	4-formylcinnamic acid (RT = 7.59 min)	0.72	1.4
	7.05	175.0375	$C_{10}H_7O_3^-$	-2.0	13.6				
	7.27	175.0395	$C_{10}H_7O_3^-$	0.0	4.5				
	7.56	175.0403	$C_{10}H_7O_3^-$	0.8	7.3				
179	5.08[d]	179.0325	$C_9H_7O_4^-$	-1.9	8.4	139 135 ($-CO_2$) 121 107[g]	2-hydroxycinnamic acid (RT = 7.68 min)	1.34	2.5
	5.47	179.0327	$C_9H_7O_4^-$	-1.7	267.4				
	6.74	179.0341	$C_9H_7O_4^-$	-0.3	2.8				
	7.05	179.0320	$C_9H_7O_4^-$	-2.4	7.1				
181	4.48	181.0128	$C_8H_5O_5^-$	-0.9	3.4	163 ($-H_2O$) 137 ($-CO_2$)[g] 93 ($-2CO_2$)	5-hydroxyisophthalic acid (RT = 5.74 min)	2.32	4.4
	4.62	181.0146	$C_8H_5O_5^-$	0.9	4.6				
	5.30[d]	181.0128	$C_8H_5O_5^-$	-0.9	13.5				
182	6.20	182.0096	$C_7H_4NO_5^-$	0.7	0.6	152 (-NO) 138 ($-CO_2$)[g]	3-hydroxy-4-nitrobenzoic acid (RT = 7.28 min)	0.35	0.7
	6.81[d]	182.0072	$C_7H_4NO_5^-$	-1.7	3.0				
188	6.50	188.0336	$C_{10}H_6NO_3^-$	-1.2	11.4	158 (-NO)[g] 145	4-nitro-1-naphthol (RT = 9.35 min)	0.18	0.3
	6.98	188.0367	$C_{10}H_6NO_3^-$	1.9	60.4				
	7.30	188.0310	$C_{10}H_6NO_3^-$	-3.8	7.6				
	7.58	188.0341	$C_{10}H_6NO_3^-$	-0.7	1.5				
	9.36[d]	188.0326	$C_{10}H_6NO_3^-$	-2.2	40.6				
	9.51	188.0357	$C_{10}H_6NO_3^-$	0.9	3.1				

TABLE 2S: continued

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
191	5.91	191.0356	$C_{10}H_7O_4^-$	1.2	808.2	173 ($-H_2O$) 147 ($-CO_2$)[g] 131 119	2-hydroxycinnamic acid (RT = 7.68 min)	1.02	1.9
	6.13	191.0342	$C_{10}H_7O_4^-$	-0.2	4.7				
	6.17	191.0348	$C_{10}H_7O_4^-$	0.4	17.0				
	6.30	191.0342	$C_{10}H_7O_4^-$	-0.2	9.4				
	6.54	191.0322	$C_{10}H_7O_4^-$	-2.2	11.4				
	6.69[d]	191.0346	$C_{10}H_7O_4^-$	0.2	31.5				
	7.33	191.0354	$C_{10}H_7O_4^-$	1.0	18.8				
	7.76	191.0339	$C_{10}H_7O_4^-$	-0.5	30.5				
193	4.11[d]	193.0128	$C_9H_5O_5^-$	-0.9	1.8	175 ($-H_2O$) 165 ($-CO$) 149 ($-CO_2$)[g] 121 105 ($-2CO_2$)	1,2,4-benzenetricarboxylic acid (RT = 4.69 min)	0.38	0.7
	5.92	193.0131	$C_9H_5O_5^-$	-0.6	95.9				
193	4.72[d]	193.0511	$C_{10}H_9O_4^-$	1.0	164.5	[e]	[f]		
	5.34	193.0527	$C_{10}H_9O_4^-$	2.6	106.3				
195	4.40	195.0312	$C_9H_7O_5^-$	1.9	15.5	177 ($-H_2O$) 163 151 ($-CO_2$)[g]	1,2,4-benzenetricarboxylic acid (RT = 4.69 min)	0.34	0.6
	4.95[d]	195.0266	$C_9H_7O_5^-$	-2.7	106.6				
	6.23	195.0301	$C_9H_7O_5^-$	0.8	29.7				
	6.38	195.0275	$C_9H_7O_5^-$	-1.8	7.6				
196	5.87	196.0282	$C_8H_6NO_5^-$	3.6	12.7	[e]	[f]		
196	8.60	196.0605	$C_9H_{10}NO_4^-$	-0.5	12.4	[e]	[f]		

TABLE 2S: continued

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
197	4.68	197.0100	$C_8H_5O_6^-$	1.4	6.5	167 153 ($-CO_2$)[g] 109 ($-2CO_2$)	5-hydroxyisophthalic acid (RT = 5.74 min)	0.06	0.1
204	8.99[d]	204.0271	$C_{10}H_6NO_4^-$	-2.6	5.5	189 174 (-NO)[g]	4-nitro-1-naphthol (RT = 9.35 min)	0.23	0.4
	9.58	204.0270	$C_{10}H_6NO_4^-$	-2.7	22.2	143			
206	6.50	206.0482	$C_{10}H_8NO_4^-$	2.9	45.7	188 ($-H_2O$)[g]	[f]		
	6.99[d]	206.0442	$C_{10}H_8NO_4^-$	-1.1	0.8	177			
	7.29	206.0452	$C_{10}H_8NO_4^-$	-0.1	15.3	161 145			
	7.58	206.0455	$C_{10}H_8NO_4^-$	0.2	16.3	133			
207	4.90	207.0320	$C_{10}H_7O_5^-$	2.7	82.1	189 ($-H_2O$) 163 ($-CO_2$)[g] 135 119 ($-2CO_2$)	2-hydroxycinnamic acid (RT = 7.68 min)	1.25	2.3
	5.25	207.0291	$C_{10}H_7O_5^-$	-0.2	101.3				
	5.39[d]	207.0293	$C_{10}H_7O_5^-$	-1.5	56.5				
	6.38	207.0307	$C_{10}H_7O_5^-$	-0.4	71.9				
	6.74	207.0283	$C_{10}H_7O_5^-$	-1.0	4.5				

TABLE 2S: continued

$[M - H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M - H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
209	4.67	209.0441	$C_{10}H_9O_5^-$	-0.9	25.0	191 ($-H_2O$) 179 165 ($-CO_2$)[g] 147 121 ($-2CO_2$)	1,2,4-benzenetricarboxylic acid (RT = 4.69 min)	0.01	0.0
238	6.50	238.0371	$C_{10}H_8NO_6^-$	1.9	64.4	220 ($-H_2O$) 194 ($-CO_2$)[g]	[f]		
	7.13	238.0353	$C_{10}H_8NO_6^-$	0.1	2.2				
	7.93[d]	238.0321	$C_{10}H_8NO_6^-$	-3.1	4.9				
total identified SOA mass ($\mu g/m^3$)					14.68				
% SOA mass closure					27.55				

[a] Proposed chemical structures for some of the $[M - H]^-$ ions listed in this table can be found in Table 3.

[b] RT = retention time of SOA constituent as measured by the UPLC/(-)ESI-TOFMS technique.

[c] Major product ions from the MS^2 analyses from the HPLC/(-)ESI-ITMS technique are only provided for the most abundant isomer associated with each [M - H]- ion.

[d] Designates the most abundant isomer for the $[M - H]^-$ ion listed.

[e] The parent $[M - H]^-$ ion was detected by the HPLC/(-)ESI-ITMS technique; however, not enough signal was available for MS^2 analysis.

[f] The isomers associated to this $[M - H]^-$ ion were not quantified at this time owing to the uncertainty in their respective chemical structures.

[g] This product ion was the base peak ion in the MS^2 spectrum collected from the HPLC/(-)ESI-ITMS technique.

TABLE 3S: SOA Constituents Characterized from a High-NO_x Naphthalene (Experiment 7)[a]

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
121	4.17	121.0302	$C_7H_5O_2^-$	1.2	2.2	[e]	benzoic acid (RT = 5.74 min)	0.86	1.6
	5.44	121.0301	$C_7H_5O_2^-$	1.1	3.4				
	5.70[d]	121.0285	$C_7H_5O_2^-$	-0.5	27.9				
133	5.20	133.0300	$C_8H_5O_2^-$	1.0	12.3	[e]	[f]		
137	5.29	137.2520	$C_7H_5O_3^-$	1.3	2.3	93 ($-CO_2$)[g]	3-hydroxybenzoic acid (RT = 6.27 min)	0.61	1.1
	6.25	137.0266	$C_7H_5O_3^-$	2.7	14.3				
	7.15[d]	137.0229	$C_7H_5O_3^-$	-1.0	1.5				
138	6.20	138.0227	$C_6H_4NO_3^-$	3.6	6.5	[e]	2-nitrophenol (RT = 7.28 min)	1.10	2.0
	6.80[d]	138.0173	$C_6H_4NO_3^-$	-1.8	2.1				
	7.38	138.0212	$C_6H_4NO_3^-$	2.1	6.1				
143	8.93	143.0532	$C_{10}H_7O_1^-$	3.5	2.5	[e]	[f]		
147	6.52[d]	147.0448	$C_9H_7O_2^-$	0.2	23.7	[e]	*trans*-cinnamic acid (RT = 8.49 min)	0.19	0.4
	6.69	147.0475	$C_9H_7O_2^-$	2.9	13.2				
	6.89	147.0483	$C_9H_7O_2^-$	3.7	9.1				
	7.76	147.0477	$C_9H_7O_2^-$	3.1	2.5				
149	4.16	149.0253	$C_8H_5O_3^-$	1.4	0.7	121 (-CO) 107	3-formylbenzoic acid (RT = 6.81 min)	0.53	1.0
	6.06[d]	149.0233	$C_8H_5O_3^-$	-0.6	12.1	105 ($-CO_2$)[g]			
154	6.62	154.0162	$C_6H_4NO_4^-$	2.2	0.9	[e]	2-nitrophenol (RT = 7.28 min)	0.97	1.8

TABLE 3S: continued

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
159	6.50	159.0475	$C_{10}H_7O_2^-$	2.9	247.7	[e]	[f]		
	7.30	159.0478	$C_{10}H_7O_2^-$	3.2	238.2				
	7.59	159.0487	$C_{10}H_7O_2^-$	4.1	178.9				
	8.02	159.0493	$C_{10}H_7O_2^-$	4.7	97.6				
	8.17[d]	159.0473	$C_{10}H_7O_2^-$	2.7	5.0				
163	5.36	163.0402	$C_9H_7O_3^-$	0.7	10.5	135 (-CO) 145 ($-H_2O$) 119 ($-CO_2$)[g]	2-hydroxycinnamic acid (RT = 7.68 min)	0.48	0.9
	5.65	163.0407	$C_9H_7O_3^-$	1.2	197.9				
	6.67	163.0416	$C_9H_7O_3^-$	2.1	4.9				
	6.80[d]	163.0396	$C_9H_7O_3^-$	0.1	10.3				
	7.44	163.0405	$C_9H_7O_3^-$	1.0	3.6				
165	5.44	165.0174	$C_8H_5O_4^-$	-1.4	11.6	138 121 ($-CO_2$)[g]	phthalic acid (RT = 5.72 min)	0.93	1.7
	5.69[d]	165.0179	$C_8H_5O_4^-$	-0.9	7.9				
173	4.07	172.9900	$C_6H_5O_4S^-$	-0.9	1.5	109 ($-SO_2$) 93 ($-SO_3$)[g] 80	4-hydroxybenzene sulfonic acid (RT = 0.92)	0.29	0.5
173	5.62	173.0274	$C_{10}H_5O_3^-$	3.5	69.9	155 ($-H_2O$) 145 (-CO)[g] 111	[f]		
	6.76	173.0285	$C_{10}H_5O_3^-$	4.6	139.4				
	7.47[d]	173.0288	$C_{10}H_5O_3^-$	4.9	63.9				
	7.73	173.0280	$C_{10}H_5O_3^-$	4.1	172.1				
	8.92	173.0283	$C_{10}H_5O_3^-$	4.4	21.6				
	8.99	173.0269	$C_{10}H_5O_3^-$	3.0	94.3				

TABLE 3S: continued

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration (ng/m^3)	% of SOA
175	6.89	175.0398	$C_{10}H_7O_3^-$	0.3	23.2	147 (-CO)[g] 131 ($-CO_2$)	4-formylcinnamic acid (RT = 7.59 min)	0.75	1.4
	7.04[d]	175.0388	$C_{10}H_7O_3^-$	-0.7	14.6				
	7.25	175.0395	$C_{10}H_7O_3^-$	0.0	8.4				
	7.56	175.0414	$C_{10}H_7O_3^-$	1.9	25.9				
179	5.06	179.0346	$C_9H_7O_4^-$	0.2	3.1	139 135 ($-CO_2$) 121 107[g]	2-hydroxycinnamic acid (RT = 7.68 min)	0.99	1.8
	5.49	179.0331	$C_9H_7O_4^-$	-1.3	5.0				
	6.74	179.0344	$C_9H_7O_4^-$	0.0	1.0				
	7.04[d]	179.0332	$C_9H_7O_4^-$	-1.2	3.5				
181	4.47	181.0154	$C_8H_5O_5^-$	1.7	15.7	163 ($-H_2O$) 137 ($-CO_2$)[g] 93 ($-2CO_2$)	5-hydroxyisophthalic acid (RT = 5.74 min)	1.47	2.7
	4.62	181.0150	$C_8H_5O_5^-$	1.3	11.8				
	5.30[d]	181.0130	$C_8H_5O_5^-$	-0.7	5.8				
182	6.20	182.0103	$C_7H_4NO_5^-$	1.4	5.5	152 (-NO) 138 ($-CO_2$)[g]	3-hydroxy-4-nitrobenzoic acid (RT = 7.28 min)	0.33	0.6
	6.80[d]	182.0085	$C_7H_4NO_5^-$	-0.4	14.0				
188	6.96	188.0336	$C_{10}H_6NO_3^-$	-1.2	60.1	158 (-NO)[g] 145	4-nitro-1-naphthol (RT = 9.35 min)	0.25	0.5
	7.28	188.0336	$C_{10}H_6NO_3^-$	-1.2	524.3				
	7.58	188.0355	$C_{10}H_6NO_3^-$	0.7	50.2				
	9.36[d]	188.0330	$C_{10}H_6NO_3^-$	-1.8	25.6				
	9.52	188.0352	$C_{10}H_6NO_3^-$	-0.4	0.3				

TABLE 3S: continued

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration (µg/m ^{3})	% of SOA
191	5.91	191.0357	$C_{10}H_7O_4^-$	1.3	667.9	173 ($-H_2O$) 147 ($-CO_2$)[g] 131 119	2-hydroxycinnamic acid (RT = 7.68 min)	1.06	1.9
	6.13[d]	191.0348	$C_{10}H_7O_4^-$	0.4	5.1				
	6.30	191.0360	$C_{10}H_7O_4^-$	1.6	29				
	6.52	191.0344	$C_{10}H_7O_4^-$	0.0	54.5				
	6.69	191.0345	$C_{10}H_7O_4^-$	0.1	57.2				
	7.76	191.0344	$C_{10}H_7O_4^-$	0.0	23.6				
193	4.13[d]	193.0125	$C_9H_5O_5^-$	-1.2	4.9	175 ($-H_2O$) 165 ($-CO$) 149 ($-CO_2$)[g] 121 105 ($-2CO_2$)	1,2,4-benzenetricarboxylic acid (RT = 4.69 min)	0.37	0.7
	5.91	193.0145	$C_9H_5O_5^-$	0.8	72.1				
193	4.72[d]	193.0501	$C_{10}H_9O_4^-$	2.7	190.4	[e]	[f]		
	5.33	193.0529	$C_{10}H_9O_4^-$	2.8	140				
195	4.43	195.0330	$C_9H_7O_5^-$	3.7	23.9	177 ($-H_2O$) 163 151 ($-CO_2$)[g]	1,2,4-benzenetricarboxylic acid (RT = 4.69 min)	0.45	0.8
	4.94[d]	195.0288	$C_9H_7O_5^-$	-0.5	36.2				
	6.22	195.0309	$C_9H_7O_5^-$	1.6	7.0				
	6.36	195.0286	$C_9H_7O_5^-$	-0.7	1.3				
196	5.86	196.0277	$C_8H_6NO_5^-$	3.1	2.0	[e]	[f]		
196	8.60	196.0607	$C_9H_{10}NO_4^-$	-0.3	5.6	[e]	[f]		
197	4.68	197.0114	$C_8H_5O_6^-$	2.8	10.8	167 153 ($-CO_2$)[g] 109 ($-2CO_2$)	5-hydroxyisophthalic acid (RT = 5.74 min)	0.03	0.1

TABLE 3S: continued

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
204	8.98[d]	204.0288	$C_{10}H_6NO_4^-$	-0.9	2.4	189 174 (-NO)[g]	4-nitro-1-naphthol (RT = 9.35 min)	0.25	0.5
	9.57	204.0303	$C_{10}H_6NO_4^-$	0.6	7.7	143			
206	6.51	206.0482	$C_{10}H_8NO_4^-$	2.9	79.7	188 ($-H_2O$)[g]	[f]		
	6.96[d]	206.0446	$C_{10}H_8NO_4^-$	-0.7	24.6	177			
	7.30	206.4570	$C_{10}H_8NO_4^-$	0.4	60.0	161			
	7.58	206.0443	$C_{10}H_8NO_4^-$	-1	1.4	145 133			
207	5.24	207.0312	$C_{10}H_7O_5^-$	1.9	163.7	189 ($-H_2O$)	2-hydroxycinnamic acid (RT = 7.68 min)	1.07	2.0
	5.39[d]	207.0279	$C_{10}H_7O_5^-$	-1.4	60.8	163 ($-CO_2$)[g]			
	6.36	207.0307	$C_{10}H_7O_5^-$	1.4	79.4	135			
	6.74	207.0279	$C_{10}H_7O_5^-$	-1.4	45.7	119 ($-2CO_2$)			
209	4.67	209.0489	$C_{10}H_9O_5^-$	3.9	20.7	191 ($-H_2O$) 179 165 ($-CO_2$)[g] 147 121 ($-2CO_2$)	1,2,4-benzenetricarboxylic acid (RT = 4.69 min)	0.00	0.0
238	7.13	238.0356	$C_{10}H_8NO_6^-$	0.4	3.1	220 ($-H_2O$)	[f]		
	7.93[d]	238.0337	$C_{10}H_8NO_6^-$	-1.5	2.5	194 ($-CO_2$)[g]			

total identified SOA mass ($\mu g/m^3$)	13.00
% SOA mass closure	23.75

[a] Proposed chemical structures for each $[M-H]^-$ ion listed in this table can be found in Table 3.

[b] RT = retention time of SOA constituent as measured by the UPLC/(-)ESI-TOFMS technique.

[c] Major product ions from the MS^2 analyses from the HPLC/(-)ESI-ITMS technique are only provided for the most abundant isomer associated with each $[M-H]^-$ ion.

[d] Designates the most abundant isomer for the $[M-H]^-$ ion listed.

[e] The parent $[M-H]^-$ ion was detected by the HPLC/(-)ESI-ITMS technique; however, not enough signal was available for MS^2 analysis.

[f] The isomers associated to this $[M-H]^-$ ion were not quantified at this time owing to the uncertainty in their respective chemical structures.

[g] This product ion was the base peak ion in the MS^2 spectrum collected from the HPLC/(-)ESI-ITMS technique.

TABLE 4S: SOA Constituents Characterized from a High-NO_x Naphthalene (Experiment 8) [a]

$[M - H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M - H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration (µg/m^3)	% of SOA
121	4.46	121.0285	$C_7H_5O_2^-$	-0.5	0.6	[e]	benzoic acid (RT = 5.74 min)	0.51	1.5
	5.44	121.0285	$C_7H_5O_2^-$	-0.5	1.4				
	5.71[d]	121.0258	$C_7H_5O_2^-$	-3.2	7.1				
133	5.23	133.0292	$C_8H_5O_2^-$	0.2	0.6	[e]	[f]		
137	4.48	137.0252	$C_7H_5O_3^-$	1.3	1.0	93 ($-CO_2$)[g]	3-hydroxybenzoic acid (RT = 6.27 min)	0.66	1.9
	5.31	137.0254	$C_7H_5O_3^-$	1.5	1.1				
	6.25	137.0254	$C_7H_5O_3^-$	1.5	10.1				
	7.20[d]	137.0204	$C_7H_5O_3^-$	-3.5	6.6				
138	6.22	138.0220	$C_6H_4NO_3^-$	2.9	1.4	[e]	2-nitrophenol (RT = 7.28 min)	0.11	0.3
	6.84[d]	138.0205	$C_6H_4NO_3^-$	1.4	0.5				
	7.38	138.0209	$C_6H_4NO_3^-$	1.8	2.7				
143	8.75	143.0536	$C_{10}H_7O_1^-$	3.9	2.9	[e]	[f]		
	8.93[d]	143.0505	$C_{10}H_7O_1^-$	0.8	1.8				
147	6.52[d]	147.0448	$C_9H_7O_2^-$	0.2	1.4	[e]	*trans*-cinnamic acid (RT = 8.49 min)	0.03	0.1
	6.67	147.0482	$C_9H_7O_2^-$	3.6	2.2				
	6.90	147.0471	$C_9H_7O_2^-$	2.5	2.2				
	7.76	147.0472	$C_9H_7O_2^-$	2.6	2.0				
149	4.17	149.0239	$C_8H_5O_3^-$	0.0	0.4	121 (-CO) 107 105 ($-CO_2$)[g]	3-formylbenzoic acid (RT = 6.81 min)	0.46	1.3
	5.92	149.0258	$C_8H_5O_3^-$	1.9	9.1				
	6.07[d]	149.0221	$C_8H_5O_3^-$	-1.8	2.2				
	6.46	149.0245	$C_8H_5O_3^-$	0.6	42.1				
154	6.64	154.0151	$C_6H_4NO_4^-$	1.1	7.9	[e]	2-nitrophenol (RT = 7.28 min)	0.08	0.25

TABLE 4S: continued

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
159	6.50	159.0466	$C_{10}H_7O_2^-$	2.0	214.8	[e]	[f]		
	7.30	159.0451	$C_{10}H_7O_2^-$	0.5	138.0				
	7.58[d]	159.0462	$C_{10}H_7O_2^-$	1.6	136.0				
	8.00	159.0462	$C_{10}H_7O_2^-$	1.6	86.9				
	8.17	159.0462	$C_{10}H_7O_2^-$	1.6	32.3				
163	5.38	163.0406	$C_9H_7O_3^-$	1.1	2.1	135 (-CO) 145 ($-H_2O$) 119 ($-CO_2$)[g]	2-hydroxycinnamic acid (RT = 7.68 min)	0.40	1.2
	5.67	163.0391	$C_9H_7O_3^-$	-0.4	339.1				
	5.97	163.0423	$C_9H_7O_3^-$	2.8	174.7				
	6.67	163.0412	$C_9H_7O_3^-$	1.7	6.0				
	6.79[d]	163.0359	$C_9H_7O_3^-$	-3.6	6.7				
	7.44	163.0422	$C_9H_7O_3^-$	2.7	19.6				
165	5.44	165.0174	$C_8H_5O_4^-$	-1.4	5.5	138 121 ($-CO_2$)[g]	phthalic acid (RT = 5.72 min)	1.06	3.1
	5.72[d]	165.0158	$C_8H_5O_4^-$	-3.0	19.2				
173	4.08	172.9903	$C_6H_5O_4S^-$	-0.6	1.3	109 ($-SO_2$) 93 ($-SO_3$)[g] 80	4-hydroxybenzene sulfonic acid (RT = 0.92)[h]	0.18	0.5

TABLE 4S: continued

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
173	5.63	173.0269	$C_{10}H_5O_3^-$	3.0	71.7	155 ($-H_2O$) 145 (-CO)[g] 111	[f]		
	6.80	173.0247	$C_{10}H_5O_3^-$	0.8	77.8				
	7.30	173.0268	$C_{10}H_5O_3^-$	2.9	185.5				
	7.48	173.0252	$C_{10}H_5O_3^-$	1.3	48.9				
	7.73[d]	173.0257	$C_{10}H_5O_3^-$	1.8	74.4				
	8.92	173.0237	$C_{10}H_5O_3^-$	-0.2	16.1				
	8.99	173.0263	$C_{10}H_5O_3^-$	2.4	15.8				
175	6.89[d]	175.0376	$C_{10}H_7O_3^-$	-1.9	19.3	147 (-CO)[g] 131 ($-CO_2$)	4-formylcinnamic acid (RT = 7.59 min)	0.58	1.7
	7.04	175.0394	$C_{10}H_7O_3^-$	-0.1	6.4				
	7.27	175.0399	$C_{10}H_7O_3^-$	0.4	8.6				
	7.56	175.0391	$C_{10}H_7O_3^-$	-0.4	0.3				
179	5.09	179.0329	$C_9H_7O_4^-$	-1.5	2.4	139 135 ($-CO_2$) 121 107[g]	2-hydroxycinnamic acid (RT = 7.68 min)	1.13	3.3
	5.48	179.0323	$C_9H_7O_4^-$	-2.1	100.4				
	6.74	179.0348	$C_9H_7O_4^-$	0.4	0.2				
	7.04[d]	179.0324	$C_9H_7O_4^-$	-2.0	22.6				
181	4.48	181.0143	$C_8H_5O_5^-$	0.6	4.8	163 ($-H_2O$) 137 ($-CO_2$)[g] 93 ($-2CO_2$)	5-hydroxyisophthalic acid (RT = 5.74 min)	0.99	2.9
	4.62	181.0166	$C_8H_5O_5^-$	2.9	3.8				
	5.30[d]	181.0130	$C_8H_5O_5^-$	-0.7	17.8				
182	6.22	182.0113	$C_7H_4NO_5^-$	2.4	1.0	152 (-NO) 138 ($-CO_2$)[g]	3-hydroxy-4-nitrobenzoic acid (RT = 7.28 min)	0.10	0.3
	6.81[d]	182.0066	$C_7H_4NO_5^-$	-2.3	6.1				

TABLE 4S: continued

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
188	6.50	188.0347	$C_{10}H_6NO_3^-$	-0.1	1.2	158 ($-NO$)[g] 145	4-nitro-1-naphthol (RT = 9.35 min)	0.14	0.4
	6.96	188.0319	$C_{10}H_6NO_3^-$	-2.9	37.9				
	7.28	188.0322	$C_{10}H_6NO_3^-$	-2.6	90.4				
	7.57	188.0332	$C_{10}H_6NO_3^-$	-1.6	6.7				
	9.36[d]	188.0335	$C_{10}H_6NO_3^-$	-1.3	10.2				
	9.50	188.0372	$C_{10}H_6NO_3^-$	2.4	2.6				
191	5.91	191.0356	$C_{10}H_7O_4^-$	1.2	351.9	173 ($-H_2O$) 147 ($-CO_2$)[g] 131 119	2-hydroxycinnamic acid (RT = 7.68 min)	0.79	2.3
	6.13	191.0346	$C_{10}H_7O_4^-$	0.2	3.6				
	6.18	191.0343	$C_{10}H_7O_4^-$	-0.1	14.6				
	6.30	191.0353	$C_{10}H_7O_4^-$	0.9	10.6				
	6.52	191.0336	$C_{10}H_7O_4^-$	-0.8	12.4				
	6.69[d]	191.0352	$C_{10}H_7O_4^-$	0.8	24.2				
	7.33	191.0347	$C_{10}H_7O_4^-$	0.3	4.3				
	7.76	191.0345	$C_{10}H_7O_4^-$	0.1	55.8				
193	4.14[d]	193.0118	$C_9H_5O_5^-$	-1.9	3.3	175 ($-H_2O$) 165 ($-CO$) 149 ($-CO_2$)[g] 121 105 ($-2CO_2$)	1,2,4-benzenetricarboxylic acid (RT = 4.69 min)	0.24	0.7
	5.92	193.0145	$C_9H_5O_5^-$	0.8	37.2				
193	4.72[d]	193.0512	$C_{10}H_9O_4^-$	1.1	9.6	[e]	[f]		
	5.34	193.0513	$C_{10}H_9O_4^-$	1.2	1.8				
195	4.40	195.0304	$C_9H_7O_5^-$	1.1	6.6	177 ($-H_2O$) 163 151 ($-CO_2$)[g]	1,2,4-benzenetricarboxylic acid (RT = 4.69 min)	0.25	0.7
	4.96[d]	195.0277	$C_9H_7O_5^-$	-1.6	18.4				
	6.23	195.0296	$C_9H_7O_5^-$	0.3	34.5				
	6.40	195.0280	$C_9H_7O_5^-$	-1.3	9.0				

TABLE 4S: continued

$[M - H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M - H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
196	5.86	196.0283	$C_8H_6NO_5^-$	3.7	1.6				
196	8.59	196.0634	$C_9H_{10}NO_4^-$	2.4	1.2	[e]	[f]		
204	8.99[d]	204.0292	$C_{10}H_6NO_4^-$	-0.5	6.0	189 174 (-NO)[g] 143	4-nitro-1-naphthol (RT = 9.35 min)	0.10	0.3
	9.56	204.0277	$C_{10}H_6NO_4^-$	-2.0	12.0				
206	6.50	206.0459	$C_{10}H_8NO_4^-$	0.6	70.9	188 ($-H_2O$)[g] 177 161 145 133	[f]		
	6.95[d]	206.0444	$C_{10}H_8NO_4^-$	-0.9	21.9				
	7.29	206.0452	$C_{10}H_8NO_4^-$	-0.1	7.1				
	7.57	206.0453	$C_{10}H_8NO_4^-$	0.0	7.6				
207	4.90	207.0324	$C_{10}H_7O_5^-$	3.1	55.7	189 ($-H_2O$) 163 ($-CO_2$)[g] 135 119 ($-2CO_2$)	2-hydroxycinnamic acid (RT = 7.68 min)	0.78	2.2
	5.25	207.0314	$C_{10}H_7O_5^-$	2.1	93.2				
	5.38[d]	207.0267	$C_{10}H_7O_5^-$	-2.6	43.1				
	6.37	207.0298	$C_{10}H_7O_5^-$	0.5	51.6				
	6.74	207.0286	$C_{10}H_7O_5^-$	-0.7	8.4				
238	6.50	238.0399	$C_{10}H_8NO_6^-$	4.7	45.2	220 ($-H_2O$) 194 ($-CO_2$)[g]	[f]		
	7.13[d]	238.0355	$C_{10}H_8NO_6^-$	0.3	2.5				
	7.93	238.0338	$C_{10}H_8NO_6^-$	-1.4	0.8				
total identified SOA mass ($\mu g/m^3$)					8.61				
% SOA mass closure					24.91				

[a] Proposed chemical structures for each $[M - H]^-$ ion listed in this table can be found in Table 3.

[b] RT = retention time of SOA constituent as measured by the UPLC/(-)ESI-TOFMS technique.

[c] Major product ions from the MS^2 analyses from the HPLC/(-)ESI-ITMS technique are only provided for the most abundant isomer associated with each $[M - H]^-$ ion.

[d] Designates the most abundant isomer for the $[M - H]^-$ ion listed.

[e] The parent $[M - H]^-$ ion was detected by the HPLC/(-)ESI-ITMS technique; however, not enough signal was available for MS^2 analysis.

[f] The isomers associated to this $[M - H]^-$ ion were not quantified at this time owing to the uncertainty in their respective chemical structures.

[g] This product ion was the base peak ion in the MS^2 spectrum collected from the HPLC/(-)ESI-ITMS technique.

TABLE 5S: SOA Constituents Characterized from a Low-NO_x Naphthalene (Experiment 3)[a]

$[M - H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M - H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
121	4.14	121.0302	$C_7H_5O_2^-$	1.2	0.4	[e]	benzoic acid (RT = 5.74 min)	0.84	2.0
	5.44	121.0273	$C_7H_5O_2^-$	-1.7	2.2				
	5.71[d]	121.0276	$C_7H_5O_2^-$	-1.4	9.4				
133	5.19	133.0285	$C_8H_5O_2^-$	-0.5	100.0	[e]	[f]		
137	4.43	137.0238	$C_7H_5O_3^-$	-0.1	2.6	93 ($-CO_2$)[g]	3-hydroxybenzoic acid (RT = 6.27 min)	1.55	3.7
	4.62	137.0247	$C_7H_5O_3^-$	0.8	3.9				
	5.28	137.0211	$C_7H_5O_3^-$	-2.8	6.0				
	6.26	137.0253	$C_7H_5O_3^-$	1.4	2.0				
	7.18[d]	137.0232	$C_7H_5O_3^-$	-0.7	4.6				
147	6.52[d]	147.0438	$C_9H_7O_2^-$	-0.8	9.3	[e]	*trans*-cinnamic acid (RT = 8.49 min)	0.19	0.5
	7.76	147.0468	$C_9H_7O_2^-$	2.2	4.3				
149	4.14	149.0227	$C_8H_5O_3^-$	-1.2	6.2	121 (-CO) 107 105 ($-CO_2$)[g]	3-formylbenzoic acid (RT = 6.81 min)	1.18	2.8
	4.57	149.0255	$C_8H_5O_3^-$	1.6	16.9				
	4.84	149.0244	$C_8H_5O_3^-$	0.5	9.8				
	5.91	149.0222	$C_8H_5O_3^-$	-1.7	44.0				
	5.99	149.0227	$C_8H_5O_3^-$	-1.2	45.8				
	6.07[d]	149.0219	$C_8H_5O_3^-$	-2.0	8.3				
	6.45	149.0239	$C_8H_5O_3^-$	-1.7	16.8				
159	8.17	159.0465	$C_{10}H_7O_2^-$	1.9	29.1	[e]	[f]		

TABLE 5S: continued

[M – H]$^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product [M – H]$^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration (μg/m^3)	% of SOA
163	5.24	163.0405	$C_9H_7O_3^-$	1.0	4.2	135 (-CO) 145 (-H_2O) 119 (-CO_2)[g]	2-hydroxycinnamic acid (RT = 7.68 min)	0.88	2.1
	5.38	163.0382	$C_9H_7O_3^-$	-1.3	1.8				
	5.45	163.0380	$C_9H_7O_3^-$	-1.5	466.8				
	5.65	163.0381	$C_9H_7O_3^-$	-1.4	1853.2				
	5.96	163.0410	$C_9H_7O_3^-$	1.5	5.7				
	6.38	163.0409	$C_9H_7O_3^-$	1.4	10.1				
	6.67	163.0401	$C_9H_7O_3^-$	0.6	0.8				
	6.79[d]	163.0385	$C_9H_7O_3^-$	-1.0	13.1				
	7.24	163.0418	$C_9H_7O_3^-$	2.3	2.8				
165	5.44	165.0170	$C_8H_5O_4^-$	-1.8	14.4	138 121 (-CO_2)[g]	phthalic acid (RT = 5.72 min)	2.11	5.0
	5.70[d]	165.0151	$C_8H_5O_4^-$	-3.7	40.0				
173	6.81[d]	173.0258	$C_{10}H_5O_3^-$	1.3	43.5	[e]	[f]		
	7.73	173.0268	$C_{10}H_5O_3^-$	3.1	66.2				
175	4.56	175.0403	$C_{10}H_7O_3^-$	0.8	156.9	147 (-CO)[g] 131 (-CO_2)	4-formylcinnamic acid (RT = 7.59 min)	0.17	0.4
	4.71	175.0395	$C_{10}H_7O_3^-$	1.1	416.8				
	5.01	175.0443	$C_{10}H_7O_3^-$	4.8	137.7				
	5.16	175.0427	$C_{10}H_7O_3^-$	3.2	17.5				
	5.36	175.0416	$C_{10}H_7O_3^-$	2.1	77.2				
	5.50	175.0424	$C_{10}H_7O_3^-$	2.9	5.2				
	5.60	175.0434	$C_{10}H_7O_3^-$	3.9	42.4				
	6.90[d]	175.0413	$C_{10}H_7O_3^-$	1.8	19.8				
	7.56	175.0412	$C_{10}H_7O_3^-$	1.7	4.8				

TABLE 5S: continued

[M – H]$^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product [M - H]$^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration (μg/m^3)	% of SOA
179	5.10	179.0328	$C_9H_7O_4^-$	-1.6	44.9	139 135 (-CO_2) 121 107[g]	2-hydroxycinnamic acid (RT = 7.68 min)	1.88	4.5
	5.49	179.0324	$C_9H_7O_4^-$	-2.0	13.1				
	5.96	179.0365	$C_9H_7O_4^-$	2.1	5.9				
	6.21	179.0332	$C_9H_7O_4^-$	-1.2	51.4				
	6.74	179.0334	$C_9H_7O_4^-$	-1.0	5.2				
	6.81	179.0313	$C_9H_7O_4^-$	-3.1	7.4				
	7.04[d]	179.0320	$C_9H_7O_4^-$	-2.4	17.3				
181	4.41[d]	181.0126	$C_8H_5O_5^-$	-1.1	4.5	163 (-H_2O) 137 (-CO_2)[g] 93 (-2CO_2)	5-hydroxyisophthalic acid (RT = 5.74 min)	4.13	9.8
	4.61	181.0127	$C_8H_5O_5^-$	-1.0	11.5				
	4.87	181.0140	$C_8H_5O_5^-$	0.3	3.9				
	5.28	181.0119	$C_8H_5O_5^-$	-1.8	21.3				
191	5.01	191.0378	$C_{10}H_7O_4^-$	3.4	27.2	173 (-H_2O) 147 (-CO_2)[g] 131 119	2-hydroxycinnamic acid (RT = 7.68 min)	0.44	1.1
	5.21	191.0364	$C_{10}H_7O_4^-$	2.0	18.4				
	5.63	191.0352	$C_{10}H_7O_4^-$	0.8	14.6				
	5.93	191.0363	$C_{10}H_7O_4^-$	1.9	1398.0				
	6.13	191.0354	$C_{10}H_7O_4^-$	1.0	22.3				
	6.30	191.0365	$C_{10}H_7O_4^-$	2.1	44.1				
	6.52[d]	191.0327	$C_{10}H_7O_4^-$	-1.7	19.1				
	6.67	191.0372	$C_{10}H_7O_4^-$	2.8	23.4				
	7.76	191.0344	$C_{10}H_7O_4^-$	0.0	43.2				

TABLE 5S: continued

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
193	4.11[d]	193.0136	$C_9H_5O_5^-$	-0.1	43.6	175 ($-H_2O$) 165 (-CO) 149 ($-CO_2$)[g] 121 105 ($-2CO_2$)	1,2,4-benzenetricarboxylic acid (RT = 4.69 min)	0.41	1.0
	5.91	193.0099	$C_9H_5O_5^-$	-3.8	574.9				
193	4.57	193.0516	$C_{10}H_9O_4^-$	1.5	146.0	[e]	[f]		
	7.69[d]	193.0514	$C_{10}H_9O_4^-$	1.3	3.2				
195	4.33	195.0293	$C_9H_7O_5^-$	0.0	83.8	177 ($-H_2O$) 163 151 ($-CO_2$)[g]	1,2,4-benzenetricarboxylic acid (RT = 4.69 min)	0.54	1.3
	4.65	195.0306	$C_9H_7O_5^-$	1.3	740.2				
	4.96[d]	195.0288	$C_9H_7O_5^-$	-0.5	24.4				
	5.88	195.0284	$C_9H_7O_5^-$	-0.9	36.7				
	6.23	195.0282	$C_9H_7O_5^-$	-1.1	36.3				
	6.37	195.0273	$C_9H_7O_5^-$	-2.0	9.6				
197	4.12	197.0098	$C_8H_5O_6^-$	1.2	12.0	167 153 ($-CO_2$)[g] 109 ($-2CO_2$)	5-hydroxyisophthalic acid (RT = 5.74 min)	1.48	3.5
	4.61	197.0089	$C_8H_5O_6^-$	0.3	9.4				
	4.81[d]	197.0064	$C_8H_5O_6^-$	-2.2	2.8				
197	4.33	197.0451	$C_9H_9O_5^-$	0.1	11.8	[e]	5-hydroxyisophthalic acid (RT = 5.74 min)	0.07	0.2
	5.29[d]	197.0474	$C_9H_9O_5^-$	2.4	3.5				

TABLE 5S: continued

$[M - H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M - H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
207	4.57	207.0275	$C_{10}H_7O_5^-$	-1.8	232.2	189 ($-H_2O$) 163 ($-CO_2$)[g] 135 119 ($-2CO_2$)	2-hydroxycinnamic acid (RT = 7.68 min)	1.86	4.4
	5.24	207.0283	$C_{10}H_7O_5^-$	-1.0	467.0				
	5.36	207.0277	$C_{10}H_7O_5^-$	-1.6	11.2				
	5.45[d]	207.0292	$C_{10}H_7O_5^-$	-0.1	27.2				
	6.36	207.0269	$C_{10}H_7O_5^-$	-2.4	69.7				
	6.74	207.0265	$C_{10}H_7O_5^-$	-2.8	48.7				
209	4.13	209.0098	$C_9H_5O_6^-$	1.2	137.3	191 ($-H_2O$) 179 165 ($-CO_2$)[g] 147 121 ($-2CO_2$)	1,2,4-benzenetricarboxylic acid (RT = 4.69 min)	0.19	0.5
	4.65[d]	209.0110	$C_9H_5O_6^-$	2.4	204.8				
	5.00	209.0122	$C_9H_5O_6^-$	3.6	63.5				
	5.43	209.0119	$C_9H_5O_6^-$	3.3	250.2				
209	5.19[d]	209.0439	$C_{10}H_9O_5^-$	-1.1	16.9	[e]	[f]		
	6.07	209.0457	$C_{10}H_9O_5^-$	0.7	9.3				
	6.52	209.0450	$C_{10}H_9O_5^-$	2.2	6.2				
	7.14	209.0465	$C_{10}H_9O_5^-$	1.5	19.1				

total identified SOA mass ($\mu g/m^3$)	17.92
% SOA mass closure	42.71

[a] Proposed chemical structures for some of the $[M - H]^-$ ions listed in this table can be found in Table 3.

[b] RT = retention time of SOA constituent as measured by the UPLC/(-)ESI-TOFMS technique.

[c] Major product ions from the MS^2 analyses from the HPLC/(-)ESI-ITMS technique are only provided for the most abundant isomer associated to each $[M - H]^-$ ion.

[d] Designates the most abundant isomer for the $[M - H]^-$ ion listed.

[e] The parent $[M - H]^-$ ion was detected by the HPLC/(-)ESI-ITMS technique; however, not enough signal was available for MS^2 analysis.

[f] The isomers associated to this $[M - H]^-$ ion were not quantified at this time owing to the uncertainty in their respective chemical structures.

[g] This product ion was the base peak ion in the MS^2 spectrum collected from the HPLC/(-)ESI-ITMS technique.

TABLE 6S: SOA Constituents Characterized from a Low-NO_x Naphthalene (Experiment 4) [a]

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
121	4.12	121.0282	$C_7H_5O_2^-$	-0.8	5.2	[e]	benzoic acid (RT = 5.74 min)	0.96	2.2
	5.44	121.0276	$C_7H_5O_2^-$	-1.4	1.6				
	5.70[d]	121.0266	$C_7H_5O_2^-$	-2.4	9.8				
133	5.19	133.0278	$C_8H_5O_2^-$	-1.2	107.2	[e]	[f]		
137	4.43	137.0241	$C_7H_5O_3^-$	0.2	3.4	93 ($-CO_2$)[g]	3-hydroxybenzoic acid (RT = 6.27 min)	1.49	3.5
	4.62	137.0260	$C_7H_5O_3^-$	2.1	1.1				
	5.28	137.0212	$C_7H_5O_3^-$	-2.7	7.9				
	6.26	μ137.0252	$C_7H_5O_3^-$	1.3	0.9				
	7.19[d]	137.0222	$C_7H_5O_3^-$	-1.7	15.5				
147	6.52[d]	147.0427	$C_9H_7O_2^-$	-1.9	13.1	[e]	*trans*-cinnamic acid (RT = 8.49 min)	0.30	0.7
	7.76	147.0456	$C_9H_7O_2^-$	1.0	0.4				
149	4.14	149.0217	$C_8H_5O_3^-$	-2.2	1.8	121 ($-CO$), 107, 105 ($-CO_2$)[g]	3-formylbenzoic acid (RT = 6.81 min)	1.21	2.8
	4.58	149.0256	$C_8H_5O_3^-$	1.7	18.6				
	4.84	149.0236	$C_8H_5O_3^-$	0.0	15.9				
	5.91	149.0221	$C_8H_5O_3^-$	-1.8	33.1				
	5.99	149.0232	$C_8H_5O_3^-$	-0.7	42.5				
	6.07[d]	149.0222	$C_8H_5O_3^-$	-1.7	41.3				
	6.45	149.0216	$C_8H_5O_3^-$	-2.3	17.1				
159	8.17	159.0469	$C_{10}H_7O_2^-$	2.3	0.7	[e]	[f]		

TABLE 6S: continued

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
163	5.24	163.0419	$C_9H_7O_3^-$	2.4	5.5	135 (-CO) 145 ($-H_2O$) 119 ($-CO_2$)[g]	2-hydroxycinnamic acid (RT = 7.68 min)	0.93	2.2
	5.38	163.0384	$C_9H_7O_3^-$	-1.1	5.6				
	5.45	163.0373	$C_9H_7O_3^-$	-2.2	30.3				
	5.65	163.0383	$C_9H_7O_3^-$	-1.2	529.2				
	5.96	163.0404	$C_9H_7O_3^-$	0.9	235.4				
	6.37	163.0404	$C_9H_7O_3^-$	0.9	9.4				
	6.67	163.0398	$C_9H_7O_3^-$	0.3	2.6				
	6.79[d]	163.0377	$C_9H_7O_3^-$	-1.8	4.7				
	7.24	163.0417	$C_9H_7O_3^-$	2.2	1.1				
165	5.44	165.0178	$C_8H_5O_4^-$	-1.0	19.9	138 121 ($-CO_2$)[g]	phthalic acid (RT = 5.72 min)	2.03	4.7
	5.69[d]	165.0150	$C_8H_5O_4^-$	-3.8	37.2				
173	4.26	172.9936	$C_6H_5O_4S^-$	2.7	1.8	109 ($-SO_2$) 93 ($-SO_3$)[g] 80	4-hydroxybenzene sulfonic acid (RT = 0.92)[h]	0.02	0.1
173	6.80[d]	173.0265	$C_{10}H_5O_3^-$	2.6	78.7	[e]	[f]		
	7.73	173.0264	$C_{10}H_5O_3^-$	2.5	21.2				

TABLE 6S: continued

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
175	4.55	175.0415	$C_{10}H_7O_3^-$	2.0	211.5	147 (-CO)[g] 131 ($-CO_2$)	4-formylcinnamic acid (RT = 7.59 min)	0.24	0.6
	4.72	175.0426	$C_{10}H_7O_3^-$	3.1	637.9				
	5.01	175.0437	$C_{10}H_7O_3^-$	4.2	130.1				
	5.16	175.0420	$C_{10}H_7O_3^-$	2.5	155.5				
	5.35	175.0406	$C_{10}H_7O_3^-$	1.1	87.9				
	5.50	175.0417	$C_{10}H_7O_3^-$	2.2	102.8				
	5.60	175.0424	$C_{10}H_7O_3^-$	2.9	10.8				
	6.90[d]	175.0419	$C_{10}H_7O_3^-$	2.4	26.3				
	7.56	175.0407	$C_{10}H_7O_3^-$	1.2	77.8				
179	5.10	179.0338	$C_9H_7O_4^-$	-0.6	6.7	139 135 ($-CO_2$) 121 107[g]	2-hydroxycinnamic acid (RT = 7.68 min)	1.92	4.4
	5.49	179.0330	$C_9H_7O_4^-$	-1.4	6.3				
	5.96	179.0345	$C_9H_7O_4^-$	0.1	14.0				
	6.21	179.0339	$C_9H_7O_4^-$	-0.5	72.3				
	6.74	179.0338	$C_9H_7O_4^-$	-0.6	7.2				
	6.80	179.0315	$C_9H_7O_4^-$	-2.9	11.5				
	7.04[d]	179.0332	$C_9H_7O_4^-$	-1.2	1.1				
181	4.42	181.0107	$C_8H_5O_5^-$	-3.0	5.9	163 ($-H_2O$) 137 ($-CO_2$)[g] 93 ($-2CO_2$)	5-hydroxyisophthalic acid (RT = 5.74 min)	3.71	8.6
	4.62	181.0129	$C_8H_5O_5^-$	-0.8	22.9				
	4.87	181.0146	$C_8H_5O_5^-$	0.9	9.6				
	5.28[d]	181.0122	$C_8H_5O_5^-$	-1.5	18.2				

TABLE 6S: continued

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
191	5.01	191.0374	$C_{10}H_7O_4^-$	3.0	45.2	173 ($-H_2O$) 147 ($-CO_2$)[g] 131 119	2-hydroxycinnamic acid (RT = 7.68 min)	0.51	1.2
	5.20	191.0358	$C_{10}H_7O_4^-$	1.4	18.7				
	5.62	191.0379	$C_{10}H_7O_4^-$	3.5	28.2				
	5.92	191.0358	$C_{10}H_7O_4^-$	1.4	1175.5				
	6.13	191.0347	$C_{10}H_7O_4^-$	0.3	30.3				
	6.30	191.0370	$C_{10}H_7O_4^-$	2.6	65.2				
	6.52[d]	191.0318	$C_{10}H_7O_4^-$	-2.6	24.3				
	6.67	191.0366	$C_{10}H_7O_4^-$	2.2	33.9				
	7.76	191.0323	$C_{10}H_7O_4^-$	-2.1	81.1				
193	4.09[d]	193.0122	$C_9H_5O_5^-$	-1.5	11.8	175 ($-H_2O$) 165 ($-CO$) 149 ($-CO_2$)[g] 121 105 ($-2CO_2$)	1,2,4-benzenetricarboxylic acid (RT = 4.69 min)	0.46	1.1
	5.91	193.0099	$C_9H_5O_5^-$	-3.8	548.7				
193	4.57	193.0503	$C_{10}H_9O_4^-$	0.2	181.3	[e]	[f]		
	7.69[d]	193.0502	$C_{10}H_9O_4^-$	0.1	161.7				
195	4.32	195.0281	$C_9H_7O_5^-$	-1.2	90.7	177 ($-H_2O$) 163 151 ($-CO_2$)[g]	1,2,4-benzenetricarboxylic acid (RT = 4.69 min)	0.67	1.5
	4.66	195.0304	$C_9H_7O_5^-$	1.1	654.7				
	4.95[d]	195.0274	$C_9H_7O_5^-$	-1.9	13.0				
	5.88	195.0279	$C_9H_7O_5^-$	-1.4	3.3				
	6.23	195.0287	$C_9H_7O_5^-$	-0.6	62.3				
	6.37	195.0280	$C_9H_7O_5^-$	-1.3	11.3				

TABLE 6S: continued

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
197	4.13	197.0119	$C_8H_5O_6^-$	3.3	8.5	167 153 ($-CO_2$)[g] 109 ($-2CO_2$)	5-hydroxyisophthalic acid (RT = 5.74 min)	1.12	2.6
	4.60[d]	197.0100	$C_8H_5O_6^-$	1.4	11.1				
	4.82	197.0085	$C_8H_5O_6^-$	-0.1	8.3				
197	4.33	197.0453	$C_9H_9O_5^-$	0.3	0.8	[e]	5-hydroxyisophthalic acid (RT = 5.74 min)	0.03	0.1
	5.29[d]	197.0465	$C_9H_9O_5^-$	1.5	0.4				
207	4.58	207.0262	$C_{10}H_7O_5^-$	-3.1	263.2	189 ($-H_2O$) 163 ($-CO_2$)[g] 135 119 ($-2CO_2$)	2-hydroxycinnamic acid (RT = 7.68 min)	2.13	4.9
	5.24	207.0298	$C_{10}H_7O_5^-$	0.5	594.3				
	5.36	207.0294	$C_{10}H_7O_5^-$	0.1	18.7				
	5.45[d]	207.0277	$C_{10}H_7O_5^-$	-1.6	39.4				
	6.35	207.0288	$C_{10}H_7O_5^-$	-0.5	34.2				
	6.72	207.0262	$C_{10}H_7O_5^-$	-3.1	67.1				
209	4.12	209.0098	$C_9H_5O_6^-$	1.2	134.7	191 ($-H_2O$) 179 165 ($-CO_2$)[g] 147 121 ($-2CO_2$)	1,2,4-benzenetricarboxylic acid (RT = 4.69 min)	0.23	0.5
	4.62[d]	209.0110	$C_9H_5O_6^-$	2.4	215.0				
	5.01	209.0118	$C_9H_5O_6^-$	3.2	42.1				
	5.40	209.0106	$C_9H_5O_6^-$	2.0	229.5				

TABLE 6S: continued

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
209	5.21[d]	209.0451	$C_{10}H_9O_5^-$	0.1	10.4	[e]	[f]		
	6.06	209.0463	$C_{10}H_9O_5^-$	1.3	5.9				
	6.52	209.0473	$C_{10}H_9O_5^-$	2.3	3.6				
	7.13	209.0467	$C_{10}H_9O_5^-$	1.7	9.8				
total identified SOA mass ($\mu g/m^3$)				17.97					
% SOA mass closure				41.57					

[a] Proposed chemical structures for some of the $[M-H]^-$ ions listed in this table can be found in Table 3.

[b] RT = retention time of SOA constituent as measured by the UPLC/(-)ESI-TOFMS technique.

[c] Major product ions from the MS^2 analyses from the HPLC/(-)ESI-ITMS technique are only provided for the most abundant isomer associated to each [M - H]- ion.

[d] Designates the most abundant isomer for the $[M-H]^-$ ion listed.

[e] The parent $[M-H]^-$ ion was detected by the HPLC/(-)ESI-ITMS technique; however, not enough signal was available for MS^2 analysis.

[f] The isomers associated to this $[M-H]^-$ ion were not quantified at this time owing to the uncertainty in their respective chemical structures.

[g] This product ion was the base peak ion in the MS^2 spectrum collected from the HPLC/(-)ESI-ITMS technique.

TABLE 7S: SOA Constituents Characterized from a Low-NO_x Naphthalene (Experiment 2)[a]

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
121	4.13	121.0283	$C_7H_5O_2^-$	-0.7	2.2	[e]	benzoic acid (RT = 5.74 min)	1.05	2.1
	5.44	121.0266	$C_7H_5O_2^-$	-2.4	3.3				
	5.70[d]	121.0264	$C_7H_5O_2^-$	-2.6	18.4				
133	5.19	133.0280	$C_8H_5O_2^-$	-1.0	89.5	[e]	[f]		
137	4.46	137.0233	$C_7H_5O_3^-$	-0.6	5.3	93 ($-CO_2$)[g]	3-hydroxybenzoic acid (RT = 6.27 min)	1.84	3.7
	4.61	137.0235	$C_7H_5O_3^-$	-0.4	6.0				
	5.28	137.0204	$C_7H_5O_3^-$	-3.5	5.6				
	6.27	137.0251	$C_7H_5O_3^-$	1.2	0.5				
	7.18[d]	137.0208	$C_7H_5O_3^-$	-3.1	8.1				
147	6.51[d]	147.0418	$C_9H_7O_2^-$	-2.8	7.9	[e]	*trans*-cinnamic acid (RT = 8.49 min)	0.29	0.6
	7.76	147.0453	$C_9H_7O_2^-$	0.7	2.3				
149	4.12	149.0217	$C_8H_5O_3^-$	-2.2	11.4	121 (-CO) 107 105 ($-CO_2$)[g]	3-formylbenzoic acid (RT = 6.81 min)	1.19	2.4
	4.57	149.0241	$C_8H_5O_3^-$	0.2	18.3				
	4.84	149.0241	$C_8H_5O_3^-$	0.2	14.4				
	5.91	149.0223	$C_8H_5O_3^-$	-1.6	43.9				
	5.99	149.0216	$C_8H_5O_3^-$	-2.3	37.6				
	6.07[d]	149.0217	$C_8H_5O_3^-$	-2.2	6.7				
	6.45	149.0217	$C_8H_5O_3^-$	-2.2	33.5				
159	6.40[d]	159.0667	$C_7H_{11}O_4^-$	1.0	0.4	[e]	[f]		

TABLE 7S: continued

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)
159	8.17	159.0470	$C_{10}H_7O_2^-$	2.4	20.1	[e]	[f]	
163	5.24	163.0402	$C_9H_7O_3^-$	0.7	1.7	135 (-CO) 145 ($-H_2O$) 119 ($-CO_2$)[g]	2-hydroxycinnamic acid (RT = 7.68 min)	1.17
	5.38	163.0372	$C_9H_7O_3^-$	-2.3	3.4			
	5.45	163.0366	$C_9H_7O_3^-$	-2.9	1701.7			
	5.64	163.0376	$C_9H_7O_3^-$	-1.9	4297.1			
	5.96	163.0398	$C_9H_7O_3^-$	0.3	267.2			
	6.38	163.0401	$C_9H_7O_3^-$	0.6	85.9			
	6.67	163.0385	$C_9H_7O_3^-$	-1.0	42.5			
	6.79[d]	163.0379	$C_9H_7O_3^-$	-1.6	18.0			
	7.24	163.0403	$C_9H_7O_3^-$	0.8	2.2			
165	5.44	165.0167	$C_8H_5O_4^-$	-2.1	7.1	138 121 ($-CO_2$)[g]	phthalic acid (RT = 5.72 min)	2.34
	5.69[d]	165.0150	$C_8H_5O_4^-$	-3.8	40.7			
173	4.26	172.9919	$C_6H_5O_4S^-$	1.0	1.0	109 ($-SO_2$) 93 ($-SO_3$)[g] 80	4-hydroxybenzene sulfonic acid (RT = 0.92)[h]	0.03
173	6.81[d]	173.0254	$C_{10}H_5O_3^-$	1.5	71.8	[e]	[f]	
	7.73	173.0258	$C_{10}H_5O_3^-$	1.9	22.3			

TABLE 7S: continued

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
175	4.56	175.0405	$C_{10}H_7O_3^-$	1.0	197.1	147 (-CO)[g] 131 ($-CO_2$)	4-formylcinnamic acid (RT = 7.59 min)	0.29	0.6
	4.71	175.0410	$C_{10}H_7O_3^-$	1.5	717.2				
	5.00	175.0429	$C_{10}H_7O_3^-$	3.4	136.2				
	5.16	175.0421	$C_{10}H_7O_3^-$	2.6	125.9				
	5.35	175.0416	$C_{10}H_7O_3^-$	2.1	82.9				
	5.50	175.0421	$C_{10}H_7O_3^-$	2.6	8.9				
	5.62	175.0435	$C_{10}H_7O_3^-$	4.0	50.1				
	6.90[d]	175.0391	$C_{10}H_7O_3^-$	-0.4	30.4				
	7.57	175.0406	$C_{10}H_7O_3^-$	1.1	7.6				
179	5.09[d]	179.0318	$C_9H_7O_4^-$	-2.6	8.6	139 135 ($-CO_2$) 121 107[g]	2-hydroxycinnamic acid (RT = 7.68 min)	2.35	4.8
	5.49	179.0318	$C_9H_7O_4^-$	-2.6	2.4				
	5.96	179.0358	$C_9H_7O_4^-$	0.9	5.9				
	6.21	179.0347	$C_9H_7O_4^-$	0.3	10.4				
	6.74	179.0338	$C_9H_7O_4^-$	-0.6	7.5				
	6.80	179.0305	$C_9H_7O_4^-$	-3.9	11.0				
	7.04	179.0330	$C_9H_7O_4^-$	-1.4	22.2				
181	4.42	181.0102	$C_8H_5O_5^-$	-3.5	9.3	163 ($-H_2O$) 137 ($-CO_2$)[g] 93 ($-2CO_2$)	5-hydroxyisophthalic acid (RT = 5.74 min)	4.35	8.8
	4.62	181.0127	$C_8H_5O_5^-$	-1.0	14.2				
	4.89	181.0140	$C_8H_5O_5^-$	0.3	13.4				
	5.28[d]	181.0103	$C_8H_5O_5^-$	-3.4	10.9				

TABLE 7S: continued

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
191	5.00	191.0360	$C_{10}H_7O_4^-$	1.6	100.8	173 ($-H_2O$) 147 ($-CO_2$)[g] 131 119	2-hydroxycinnamic acid (RT = 7.68 min)	0.79	1.6
	5.21	191.0356	$C_{10}H_7O_4^-$	1.2	12.3				
	5.63	191.0369	$C_{10}H_7O_4^-$	2.5	12.8				
	5.93	191.0362	$C_{10}H_7O_4^-$	1.8	1025.8				
	6.13	191.0336	$C_{10}H_7O_4^-$	-0.8	15.6				
	6.30	191.0349	$C_{10}H_7O_4^-$	0.5	62.8				
	6.52[d]	191.0305	$C_{10}H_7O_4^-$	-3.9	44.4				
	6.67	191.0350	$C_{10}H_7O_4^-$	0.6	40.0				
	7.76	191.0320	$C_{10}H_7O_4^-$	-2.4	125.6				
193	4.13[d]	193.0105	$C_9H_5O_5^-$	-3.2	23.5	175 ($-H_2O$) 165 ($-CO$) 149 ($-CO_2$)[g] 121 105 ($-2CO_2$)	1,2,4-benzenetricarboxylic acid (RT = 4.69 min)	0.50	1.0
	5.91	193.0102	$C_9H_5O_5^-$	-3.5	598.3				
193	4.57	193.0514	$C_{10}H_9O_4^-$	1.3	176.8	[e]	[f]		
	7.69[d]	193.0499	$C_{10}H_9O_4^-$	-0.2	176.4				
195	4.32	195.0288	$C_9H_7O_5^-$	-0.5	76.1	177 ($-H_2O$) 163 151 ($-CO_2$)[g]	1,2,4-benzenetricarboxylic acid (RT = 4.69 min)	0.77	1.6
	4.66	195.0315	$C_9H_7O_5^-$	2.2	663.6				
	4.95[d]	195.0295	$C_9H_7O_5^-$	0.2	3.5				
	5.89	195.0277	$C_9H_7O_5^-$	-1.6	38.1				
	6.23	195.0270	$C_9H_7O_5^-$	-2.3	34.9				
	6.38	195.0279	$C_9H_7O_5^-$	-1.4	4.2				

TABLE 7S: continued

$[M-H]^-$ ion (*m/z*)	RT[b] (min)	TOFMS measured mass	TOFMS suggested formula	error (mDa)	i-Fit	major product $[M-H]^-$ ions (*m/z*)[c]	standard used for quantification	mass concentration ($\mu g/m^3$)	% of SOA
197	4.11	197.0092	$C_8H_5O_6^-$	0.6	12.8	167 153 ($-CO_2$)[g] 109 ($-2CO_2$)	5-hydroxyisophthalic acid (RT = 5.74 min)	1.45	2.9
	4.61[d]	197.0089	$C_8H_5O_6^-$	0.3	17.6				
	4.81	197.0075	$C_8H_5O_6^-$	-1.1	3.6				
207	4.57	207.0259	$C_{10}H_7O_5^-$	-3.4	174.2	189 ($-H_2O$) 163 ($-CO_2$)[g] 135 119 ($-2CO_2$)	2-hydroxycinnamic acid (RT = 7.68 min)	2.11	4.3
	5.24	207.0282	$C_{10}H_7O_5^-$	-1.1	290.9				
	5.38	207.0280	$C_{10}H_7O_5^-$	-1.3	33.2				
	5.45[d]	207.0281	$C_{10}H_7O_5^-$	-1.2	6.1				
	6.35	207.0264	$C_{10}H_7O_5^-$	-2.9	100.5				
	6.73	207.0258	$C_{10}H_7O_5^-$	-3.5	60.7				
209	4.13	209.0091	$C_9H_5O_6^-$	0.5	106.7	191 ($-H_2O$) 179 165 ($-CO_2$)[g] 147 121 ($-2CO_2$)	1,2,4-benzenetricarboxylic acid (RT = 4.69 min)	0.22	0.4
	4.65[d]	209.0098	$C_9H_5O_6^-$	1.2	213.0				
	5.00	209.0118	$C_9H_5O_6^-$	3.2	79.3				
	5.40	209.0100	$C_9H_5O_6^-$	1.4	335.1				
209	5.19[d]	209.0429	$C_{10}H_9O_5^-$	-2.1	29.7	[e]	[f]		
	6.06	209.0447	$C_{10}H_9O_5^-$	-0.3	4.1				
	6.51	209.0463	$C_{10}H_9O_5^-$	1.3	6.6				
	7.13	209.0459	$C_{10}H_9O_5^-$	0.9	4.4				
total identified SOA mass ($\mu g/m^3$)					20.74				
% SOA mass closure					41.91				

[a] Proposed chemical structures for some of the $[M-H]^-$ ions listed in this table can be found in Table 3.

[b] RT = retention time of SOA constituent as measured by the UPLC/(-)ESI-TOFMS technique.

[c] Major product ions from the MS^2 analyses from the HPLC/(-)ESI-ITMS technique are only provided for the most abundant isomer associated to each [M - H]- ion.

[d] Designates the most abundant isomer for the $[M-H]^-$ ion listed.

[e] The parent $[M-H]^-$ ion was detected by the HPLC/(-)ESI-ITMS technique; however, not enough signal was available for MS^2 analysis.

[f] The isomers associated to this $[M-H]^-$ ion were not quantified at this time owing to the uncertainty in their respective chemical structures.

[g] This product ion was the base peak ion in the MS^2 spectrum collected from the HPLC/(-)ESI-ITMS technique.

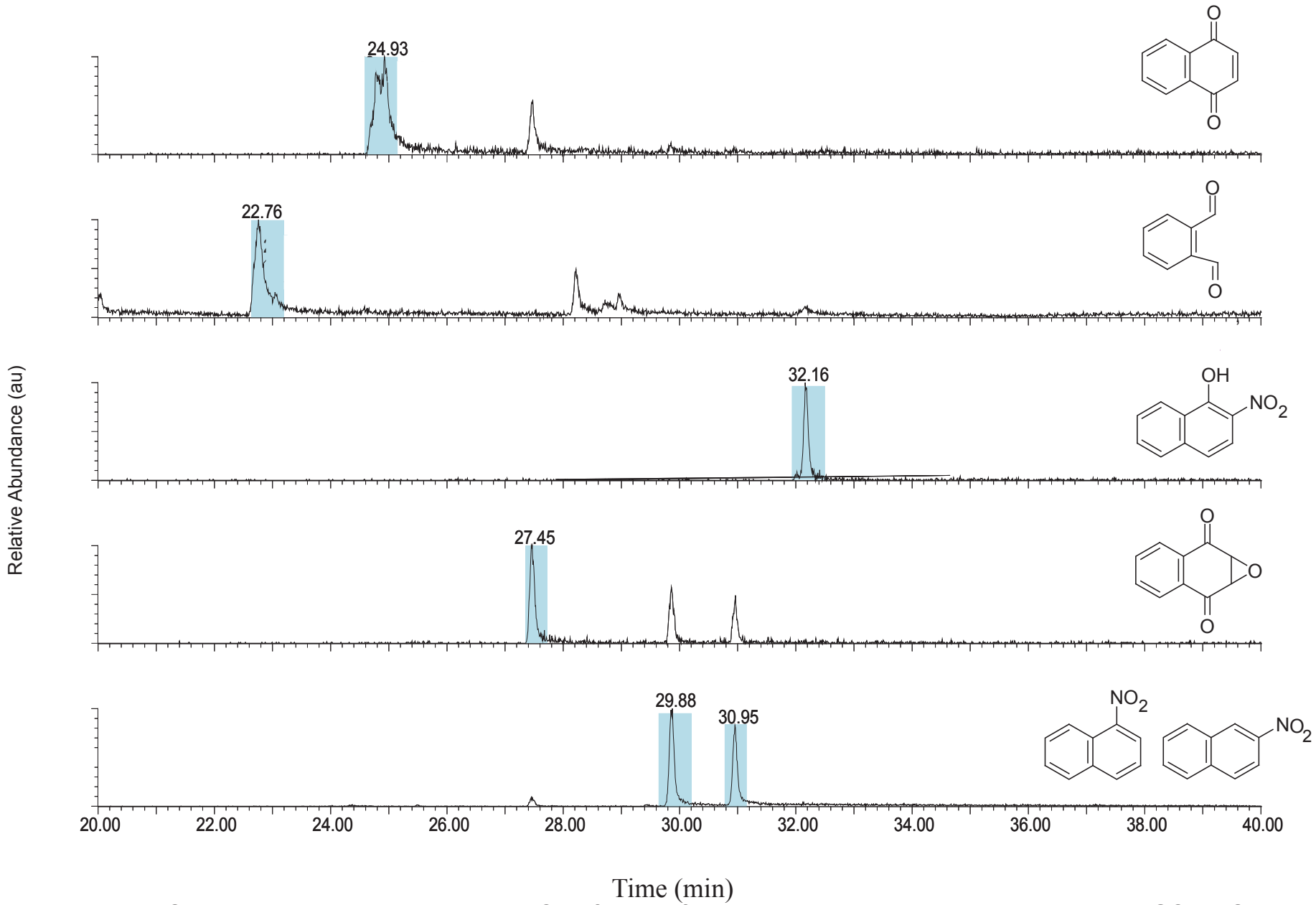

Figure 1S: Extracted ion chromatograms (EICs) of some of the photooxidation products observed by the GC/(-)ESI-TOFMS technique under high-NO_X conditions.

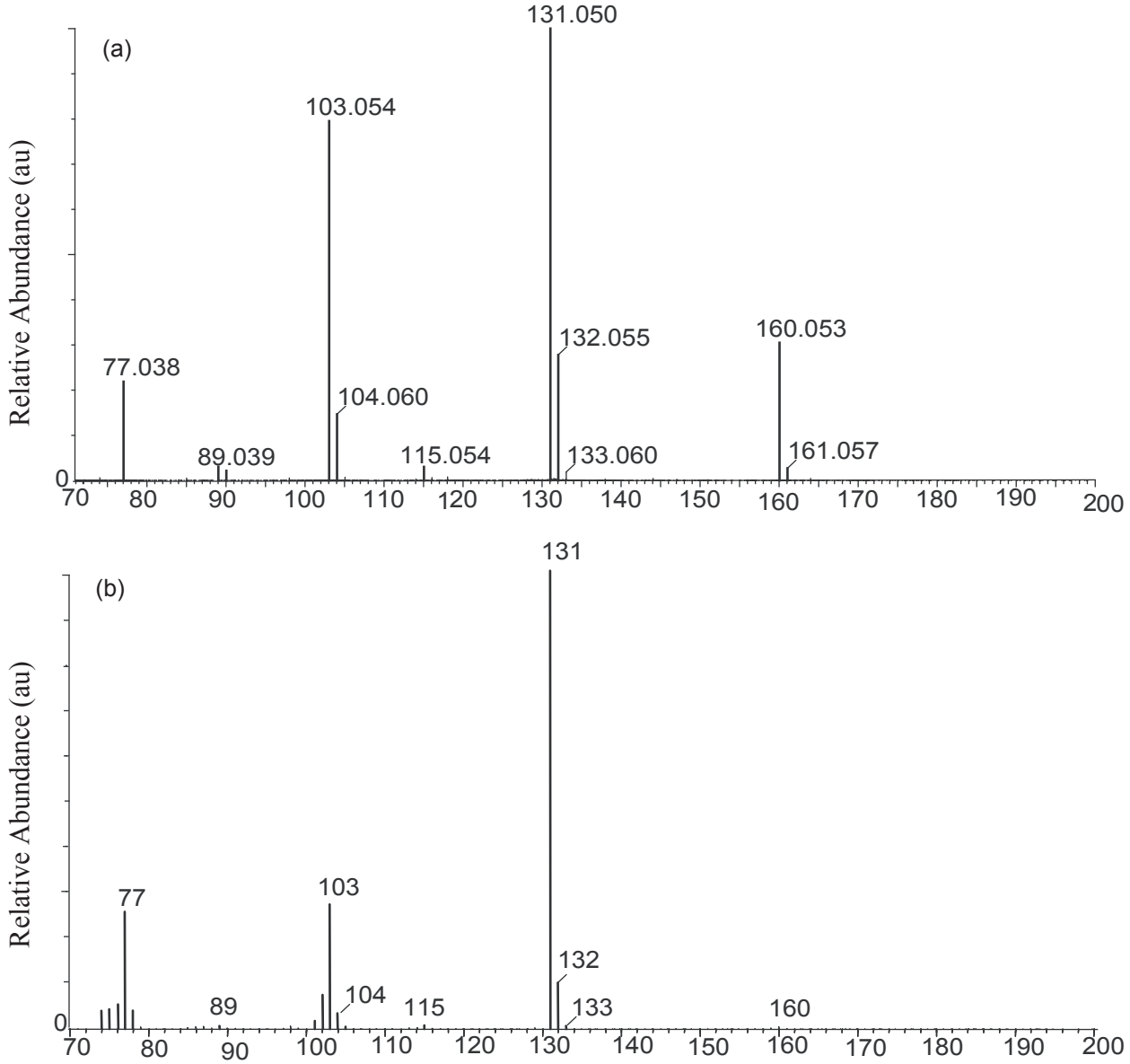

Figure 2S: a) The top panel displays a mass spectrum for *m/z* 160 detected in high- and low-NO_x experiments. b) The bottom panel shows the mass spectrum for the synthesized 2-formylcinnamaldehyde standard.

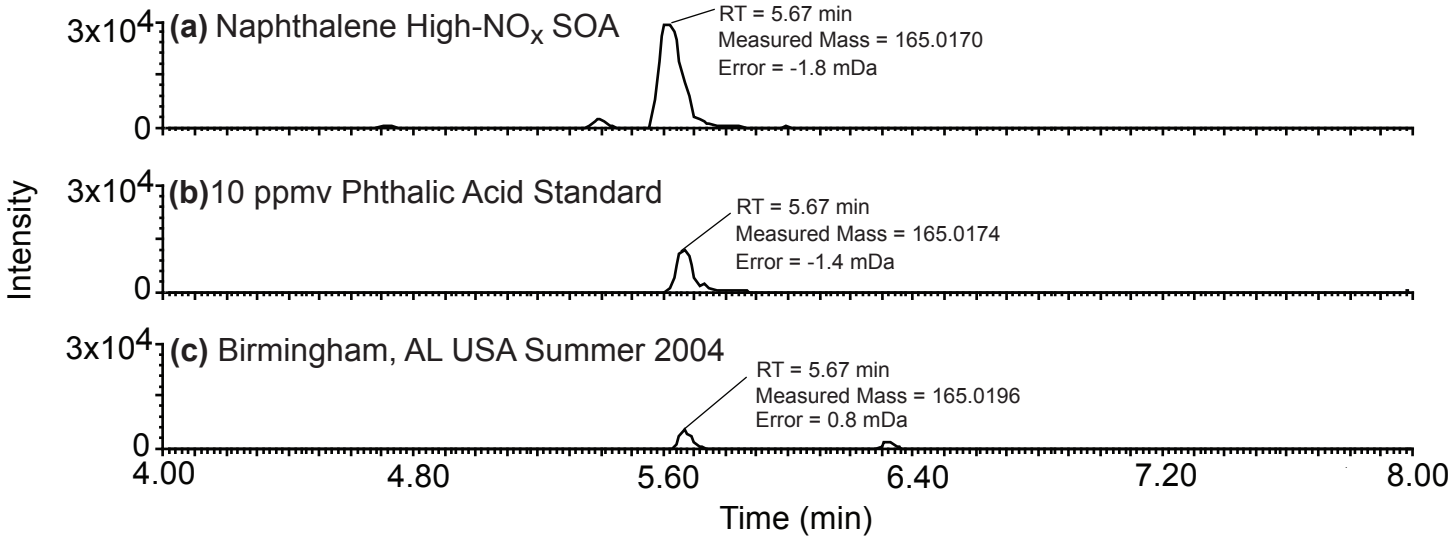

Figure 3S. UPLC/(-)ESI- TOFMS EICs of *m/z* 165. Based on the accurate mass measurements of the *m/z* 165 ions associated with each of the chromatographic peaks highlighed in panels (a) - (c), it is found they all share an elemental composition of $C_8H_5O_4^-$. Additionally, comparison of these EICs demonstrates that phthalic acid is observed in both the laboratory-generated naphthalene high-NO_x SOA and in an urban aerosol sample collected from Birmingham, AL during summertime polluted conditions. 14 ng m^{-3} of phthalic acid was measured in the urban aerosol sample collected from Birmingham,AL shown in panel (c).

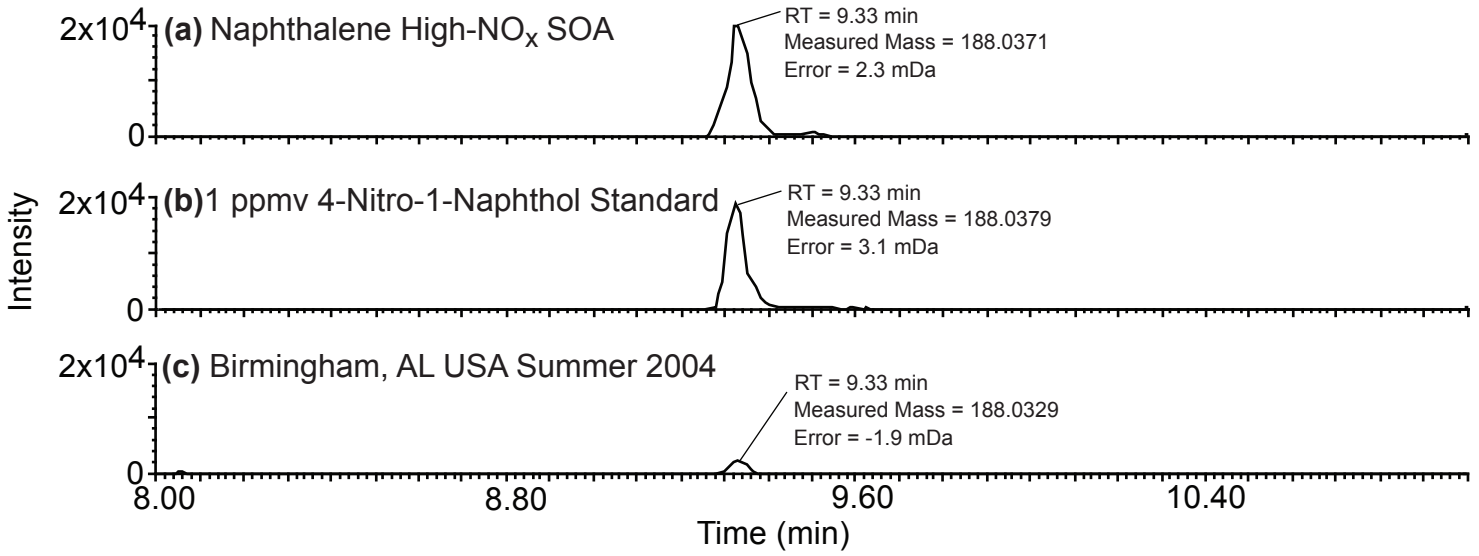

Figure 4S. UPLC/(-)ESI- TOFMS EICs of *m/z* 188. Based on the accurate mass measurements of the *m/z* 188 ions associated with each of the chromatographic peaks highlighted in panels (a) - (c), it is found they all share an elemental composition of $C_{10}H_6NO_3^-$. Additionally, comparison of these EICs demonstrate that 4-nitro-1-naphthol is observed in both the laboratory-generated naphthalene high-NO_x SOA and in the urban aerosol sample collected from Birmingham, AL during summertime polluted conditions. 1.6 ng m^{-3} of 4-nitro-1-naphthol was measured in the urban aerosol sample collected from Birmingham, AL shown in panel (c).